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## “PREDICTION IS HARD—PARTICULARLY ABOUT THE FUTURE”

—Attributed to Yogi Berra



James I. Drever

Back in 1989 I put together a model for the chemical evolution of a pit lake in a gold mine as part of an environmental-impact statement. It was a primitive affair that said basically that if you had a lot more calcite than pyrite in the wall rock the lake would not be acid and if you had a plausible amount of pyrite undergoing oxidation, adsorption would take care of the heavy metals and arsenic. Calcium and sulfate concentrations would depend on the depth to which pyrite in the wall rock underwent oxidation (for which I made an arbitrary guess) and on evaporation, which was the main control on other major solutes. I used the same general approach to estimate the composition of runoff/recharge from mine waste dumps.

When I look at recent models in permit applications, I realize that the world has changed. For pit lakes, hydrologic models of inflows and outflows have become more sophisticated, there's a model for oxygen diffusion into the pit wall, there's a model for oxygen diffusion into altering pyrite grains, there's a model for circulation and turnover in the pit lake as it fills, and there are predictions to two decimal places of the concentration of every solute over time for the next century or two. In one example, uncertainty was evaluated using Monte Carlo simulations based on uncertainties in the composition of the inflowing groundwaters. Models for the impact of mine waste on surface water and groundwater have become even more complex, and involve weather simulations, models for growth of vegetation and transpiration, models for unsaturated flow, and models for physical erosion, as well as a full set of chemical models.

What have we gained and what have we lost? On the positive side, I am sure the predictions of the more sophisticated modeling are likely to be more accurate than those of the primitive model. On the other hand, we have lost transparency—there's no realistic way an outsider can repeat the calculation as a check. The most important thing that gets lost in the process is an understanding of the uncertainties associated with the predictions. We presumably have our doubts about the two decimal places, but how confident are we in the overall prediction? In the example above, the Monte Carlo approach assumed that the only source of uncertainty in the final prediction was the estimated composition of the inflowing groundwater, which is clearly an unreasonable simplification. There are uncertainties in hydrologic models, in the models for oxygen dif-

fusion and pyrite oxidation, in the distribution of minerals in the wall rock, in the assumptions of chemical equilibrium, in the thermodynamic database, and so on.

So do we throw up our hands and say the predictions are unreliable and should be ignored? We can't predict accurately what the composition of the pit lake will be, so should we stop issuing permits until we can be 100% sure? Or should we say that permits should be issued unless we are 100% sure there *will* be a problem? I have talked about pit lakes here to illustrate an issue that faces us all as scientists and citizens. Modeling a pit lake is a vastly simpler problem than modeling the performance of a radioactive-waste repository such as Yucca Mountain (although our modeling does not include the vagaries of politics!) or modeling the response of climate to inputs of carbon dioxide. These models have in common that they are enormously complex, have uncertainties that are hard to quantify, and potentially guide enormously important policy decisions.

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I would argue that even though there are uncertainties that are hard to quantify in model predictions, these predictions represent the best estimate we have of what will happen in the future, and it makes sense to use them as a starting point for policy decisions. There is no such thing as absolute certainty about the future. This is something of a public relations challenge for us geochemists: yes, we know that the predictions have their limitations, but yes, we recognize that they are almost certainly qualitatively correct and provide a sound basis for political decisions.

To me the route to greater confidence in the model predictions is not—at least in the examples of pit lakes, mine wastes, and radioactive-waste disposal—through ever more sophisticated mathematical modeling. I think our skills at modeling have run ahead of our understanding of some of the underlying physical processes and our ability to test the models against real data from the field. Improvements will come from better understanding of the underlying physical processes, exemplified by detailed characterization of the mineral reactions that release contaminants, as discussed in this issue, and from field tests of model assumptions. We also need to be able to communicate the basic concepts that underlie the models and provide real, if qualitative, constraints: if there's much more calcite than pyrite the water will not be acidic; radioactive contaminants will not move much faster than groundwater; carbon dioxide is indeed a greenhouse gas. We should not get hung up on specific numbers, which we know are, paraphrasing Donald Rumsfeld, subject to unknown uncertainties.

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\* James I. Drever was the principal editor in charge of this issue.